

Patent claims

1. Method for designing experiments for achieving an optimization goal having the following steps:

5

A) selection of at least a first experiment from an experimental space by means of a data-driven optimizer in a computer unit,

10

B) inputting of experimentally determined experiment data of the first experiment in at least one meta layer into a computer unit,

C) use of at least one meta layer for the evaluation of the experiment data,

15

D) inputting of the experimentally determined experiment data of the first experiment into the data-driven optimizer,

E) influencing of the data-driven optimizer by the result of the evaluation in the meta layer and checking the goal achieved,

20

F) selection of at least a second experiment from the experimental space by means of the data-driven optimizer,

G) repetition of steps B) to E) for the data of the second experiment,

25

and

H) stopping the hexation on achieving the goal or repeating steps A) to F) for at least a third or subsequent experiments until the goal has been achieved.

30

2. Method according to Claim 1, the experimental space being changed, in particular restricted, displaced or enlarged by means of the optimizer and/or the meta layer before the selection of the at least one second experiment.

35

3. Method according to Claim 1 or 2, the meta layer containing a neural network and/or a hybrid model and/or a rigorous model and/or one or more data mining methods.

4. Method according to Claim 1, 2 or 3, experiments from the field of active ingredient research, materials research, catalysis research, biotechnology and/or optimization of reaction conditions being carried out in order to determine the experimental data.
5
5. Method according to one of the preceding Claims 1 to 4, the influencing of the data-driven optimizer being carried out by filtering the experiment data on the basis of the evaluation.
- 10 6. Method according to Claim 5, the filtering being carried out by means of a re-evaluation of the experiment data.
7. Method according to Claim 5, the filtering being carried out by means of weighting and/or preselection of the experiment data.
15
8. Method according to Claim 7, the weighting being carried out by means of a weighting parameter or by means of single or multiple duplication of the experiment data.
- 20 9. Method according to one of the preceding Claims 1 to 8, the optimizer having at least one core module and one module for selecting new test points.
10. Method according to Claim 9, the data-driven optimizer being influenced by influencing the module for the selection of new test points.
25
11. Method according to Claim 10, the module for selecting new test points being influenced when a threshold value is exceeded and/or by means of values predefined by a user.
- 30 12. Method according to Claim 9, the data-driven optimizer being influenced by influencing the core module.
13. Method according to Claim 12, the core module being influenced when a threshold value is exceeded and/or by means of values predefined by a user.
35
14. Computer program product for carrying out a method according to one of the preceding Claims 1 to 13.
15. Computer system for designing experiments having:

- A. a data-driven optimizer (6) for selecting at least one first experiment from an experimental space (1),
- 5 B. a meta layer (9) for the data-driven optimizer for the evaluation of experiment data determined experimentally for the first experiment, the meta layer containing a neural network and/or a hybrid model and/or a rigorous model and/or data mining methods, and the meta layer for influencing the data-driven optimizer being constructed on the basis of the result of the evaluation.
- 10
- 16. Computer system according to Claim 15, having means for filtering (13; 15) the experiment data on the basis of the evaluation.
- 15 17. Computer system according to Claim 16, the filtering means being designed to re-evaluate the experiment data.
- 18. Computer system according to Claim 16, the filtering means being designed to weight and/or preselect the experiment data.
- 20
- 19. Computer system according to one of the preceding Claims 15 to 18, the optimizer having at least one core module (16) and one module (17) for selecting new test points.
- 25 20. Computer system according to Claim 19, the meta layer being designed to influence the module for selecting new test points.
- 21. Computer system according to Claim 19, the meta layer being designed to influence the core modules.
- 30